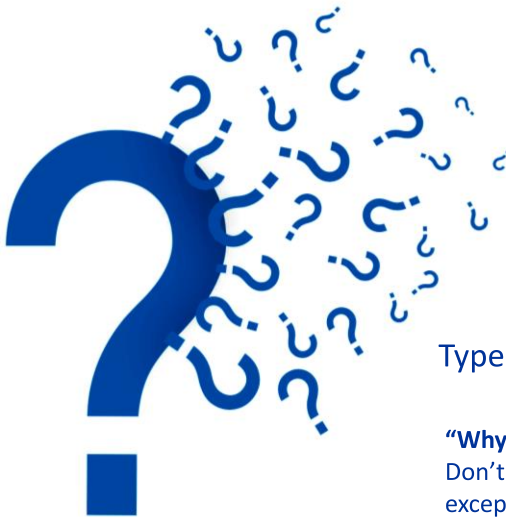
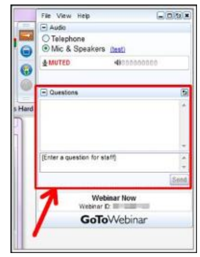
Have Questions?





Type them into questions box!

"Why am I muted?"
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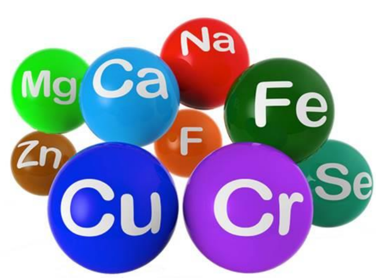

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Kathy Wall MS, Chemistry Lab Coordinator
Waubonsee Community College,
ACS member for 13 years strong!

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Upcoming ACS Webinars
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Thursday, May 25, 2017

Anti-Infectives: *Rational Approaches to the Design and Optimization*

Co-produced with the ACS Division of Medicinal Chemistry and the AAPS

Jason Sello, Associate Professor of Chemistry, Brown University

Courtney Aldrich, Associate Professor, Department of Medicinal Chemistry, University of Minnesota and Editor-in-Chief of *ACS Infectious Diseases*

Thursday, June 1, 2017

Advances in Graphene Nanotechnology: *Making the Paralyzed Walk*

Co-produced with ACS Industry Member Programs, ACS Committee on Corporation Associates, and C&EN

James Tour, W. F. Chao Professor of Chemistry, Professor of Computer Science, and Professor of Materials Science and NanoEngineering, Rice University

William Sikkema, Ph.D. Candidate, Rice University

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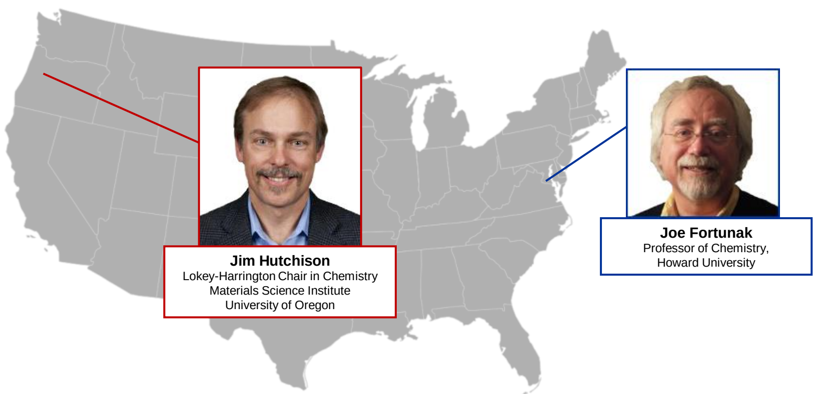
Nanomaterial Design Guided by the Principles of Green Chemistry



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This ACS Webinar is co-produced by the ACS Green Chemistry Institute

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Nanomaterial Design Guided by the Principles of Green Chemistry

Professor Jim Hutchison

Lokey-Harrington Chair in Chemistry

Materials Science Institute

University of Oregon

MSi materials science institute

UNIVERSITY OF OREGON

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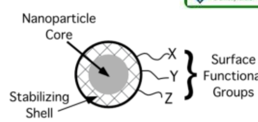
What You Will Learn

- Applying green chemistry principles and tools to nano

- Designing greener nanoscale building blocks



- Designing for product innovation and commercialization

The Promise of Nanotechnology for Society and the Environment Relies on New Properties

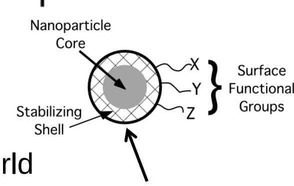
Abundant clean <u>energy</u> from the sun

High performance <u>energy storage and use</u>

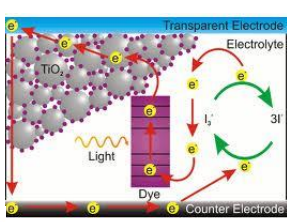
Drinkable <u>water</u> for everyone around the world

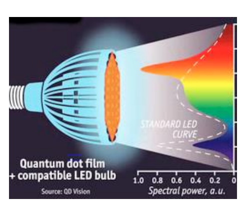
Enhanced medical <u>diagnostics and therapies</u>

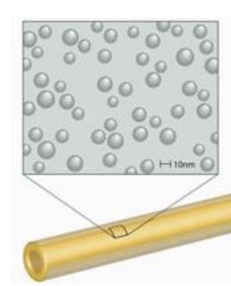
Clean, sustainable <u>chemical production</u>



Functional, nanoscale architecture!

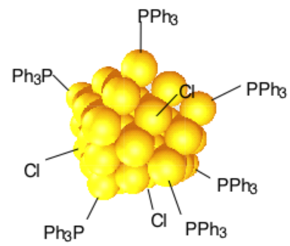






Pioneering synthesis of gold nanoparticles…effective, but not so safe/green

$$(PPh_3)AuCl \xrightarrow[\text{benzene}]{B_2H_6}$$

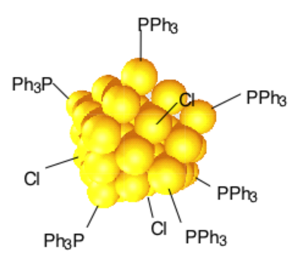


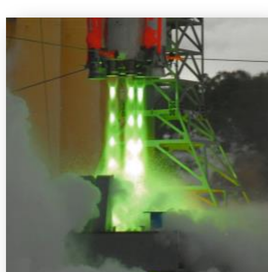
Schmid, G. *Inorg. Synth.* ***1990***, 27, 214

15

Pioneering synthesis of gold nanoparticles…effective, but not so safe/green

$$(PPh_3)AuCl \xrightarrow[\text{benzene}]{B_2H_6}$$





http://imgur.com/gallery/hWOrS

Hazardous, wasteful, low yields, batch-to-batch variation, impure samples (or unknown purity), little mechanistic knowledge to guide synthesis, expensive…

Schmid, G. *Inorg. Synth.* ***1990***, 27, 214

16

Will new properties at the nanoscale adversely impact health and/or environment?

Do new properties contribute to:

- Toxicity?
- Ecotoxicity?
- Persistence?
- Bioaccumulation?

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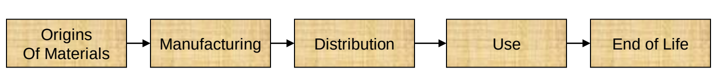
Greener nano, safer nano, sustainable nano…

Apply 12 principles of green chemistry to

- *reduce hazards and*
- *minimize impacts of production*
- *across the value chain and lifecycle of nanomaterials*

Lux Research, 2007



Molecular-level design to maximize net environmental benefits (in the context of alternatives)

McKenzie and Hutchison *Chemistry Today,* **2004**, 30
Dahl; Maddux; Hutchison *Chem. Rev.* **2007**, *107,* 2228
Hutchison *ACS Nano* **2008**, *2*, 395

18

Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

How would you describe your knowledge of green chemistry and nanotechnology?

- I have a good working knowledge of green chemistry
- I have a good working knowledge of nanotechnology
- I am knowledgeable about both green chemistry and nanotechnology
- Both green chemistry and nanotechnology are new to me

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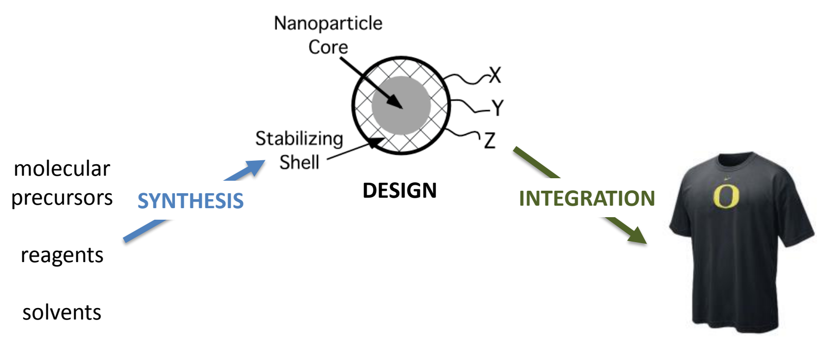
Roadmap for the rest of this webinar



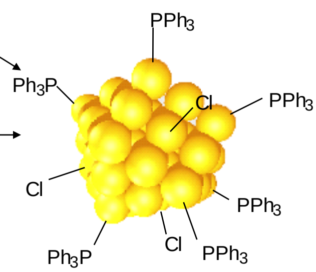
Common themes:
- Green chemistry can improve performance, lower impact
- Molecular-level understanding and design are keys to success
- Successful design improves the net benefit
- Reducing impact cannot sacrifice needed performance

20

Application of green chemistry principles to nanoparticle synthesis: Safer reagents and solvents

HAuCl$_4$ + PPh$_3$ → (ethanol) → AuCl(PPh$_3$) → (B_2H_6, C_6H_6) →

HAuCl$_4$ + PPh$_3$ → (NaBH$_4$ (10 eq), toluene/water/TOABr (1 eq)) →



Using the new method:

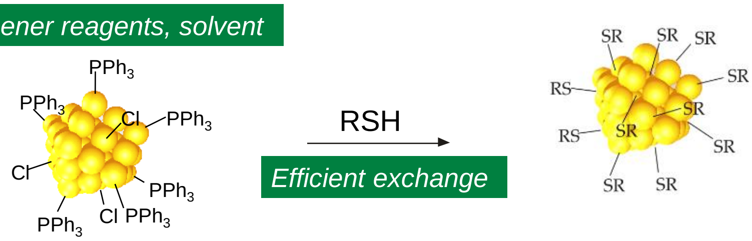
- Safer, easier, rapid preparation
- Eliminates use of diborane and benzene
- Cheaper (~ $500/g vs. “$300,000/g”)

Weare, et al. *J. Am. Chem. Soc.* **2000**, *122*, 12890.
Hutchison, et al. *Inorg. Syn*. **2004**, *34*, 228.

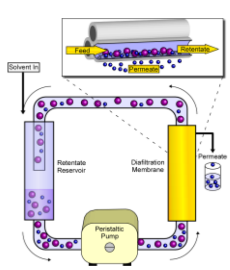
21

Developing a greener nano toolbox

Greener reagents, solvent



J. Am. Chem. Soc. **2000**, *122*, 12890; *Inorg. Syn*. **2004**, *34*, 228; *J. Am. Chem. Soc.* **1997**, *119*, 12384; *J. Phys. Chem. B* **2002**, *106*, 9979



Rapid, effective purification

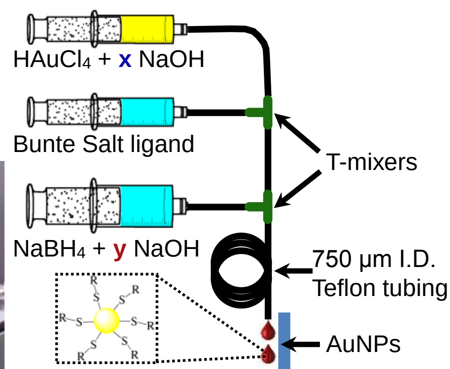
J. Am. Chem. Soc. **2006**, *128*, 3190.

Greener, cheaper, faster, better

22

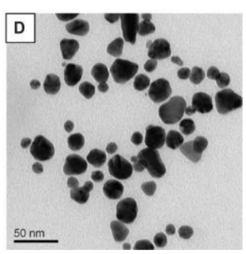
Flow chemistry, automated analysis and direct synthesis: Accelerates innovation, eliminates steps and purifications

- Precise control of core size
- Precise control of coatings
- Reproducible
- Rapid and scalable
- High yield

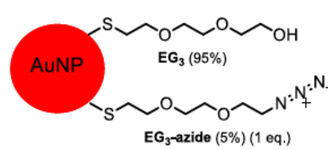


Elliott, E.W. et al., *Langmuir*, **2015**, *31*, 11886–11894

Sometimes "greener" isn't good enough



vs.



Different syntheses, different structures, different performance

Important variables:
- Size, shape, dispersity
- Dispersibility
- Targeting groups

We must evaluate performance as well as impact

Summary of greener nanosynthesis

Successful application of green chemistry to nanoscience

- Safer reagents and solvents
- Improved yields
- More efficient purification
- Fewer synthetic steps
- More mechanistic understanding to guide synthesis

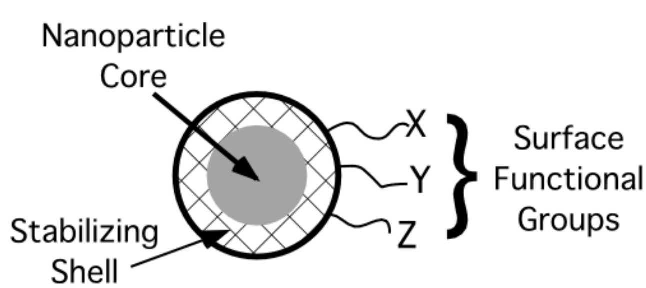
Still to do

- Further expansion of the synthetic toolbox
- Need to assess and compare performance as well as impacts

Possible to use a green route, but not produce then material you need

25

Can we design safer nanoparticles? How?



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Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

In what ways do nanoparticles differ from molecular species? (multiple correct answers possible)

- Heterogeneity of structure
- Increased surface area
- Polyvalency
- Multiple functional groups
- None of the above

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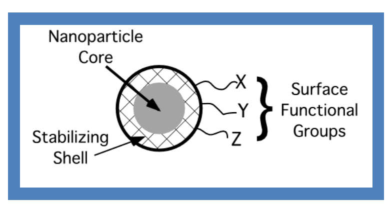
Nanomaterials are different than traditional "molecular" species or larger particles

Pronounced heterogeneity – size, shape, surface coating, purity

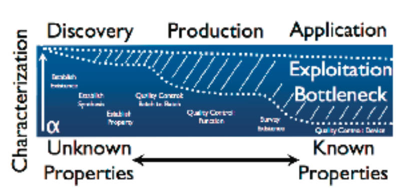
Larger size and novel 3-D structure (polyvalency)



Much higher surface areas (and higher reactivity) than larger particles

Purification challenging due to high surface area and reactivity

Characterization "bottleneck"



Richman and Hutchison *ACS Nano* **2009**, *3*, 2441-2446

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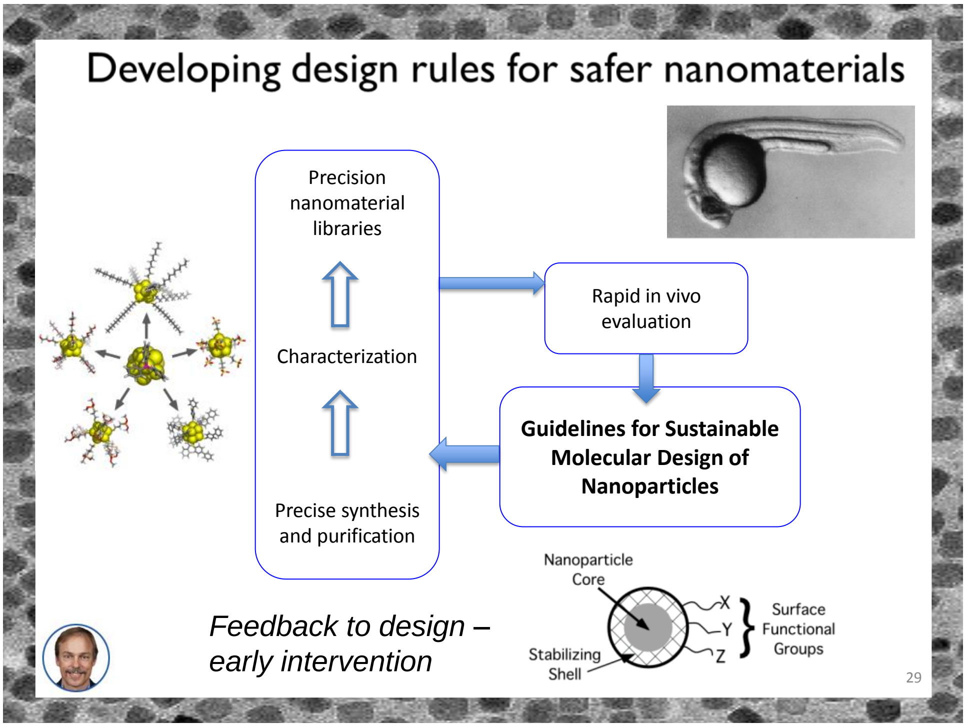
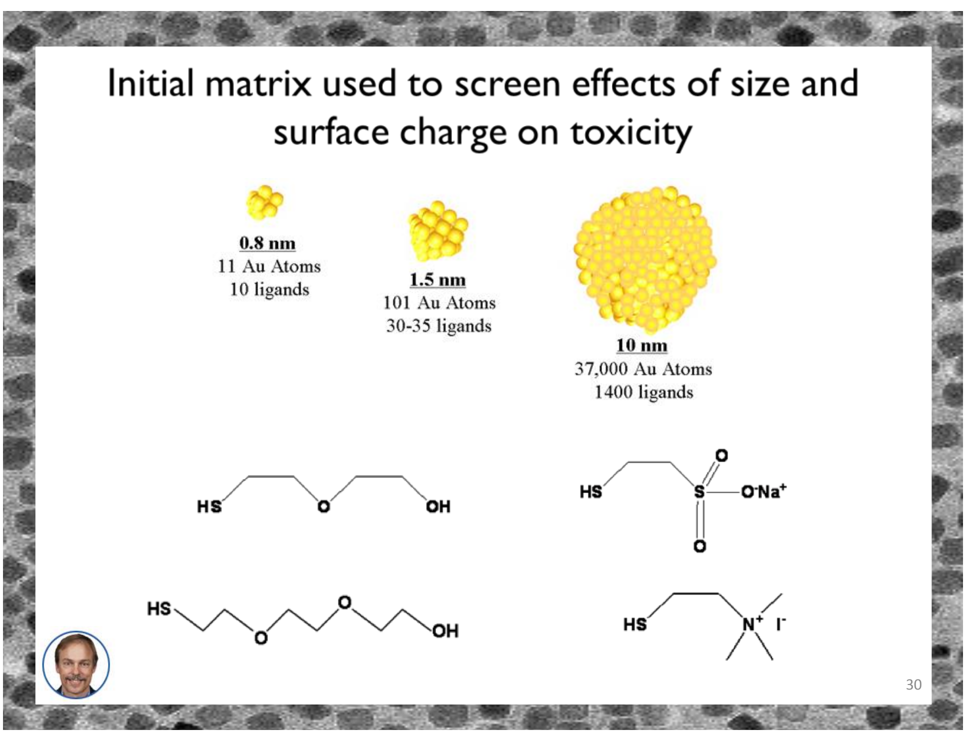
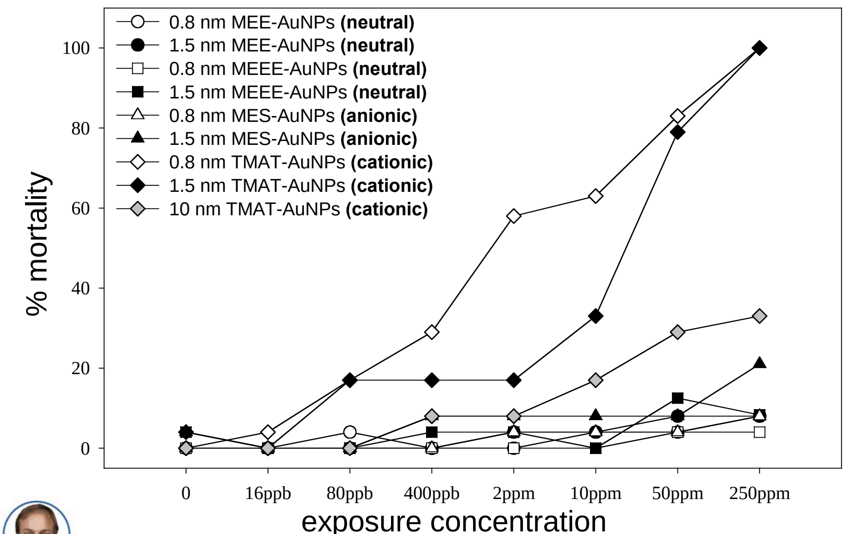

Developing design rules for safer nanomaterials
Precision nanomaterial libraries
Characterization
Precise synthesis and purification
Rapid in vivo evaluation
Guidelines for Sustainable Molecular Design of Nanoparticles
Nanoparticle Core
Stabilizing Shell
X
Y
Z
Surface Functional Groups
Feedback to design – early intervention
29


Initial matrix used to screen effects of size and surface charge on toxicity
0.8 nm
11 Au Atoms
10 ligands
1.5 nm
101 Au Atoms
30-35 ligands
10 nm
37,000 Au Atoms
1400 ligands
HS
O
OH
HS
S
O
O
O-Na+
HS
O
O
OH
HS
N+ I-
30

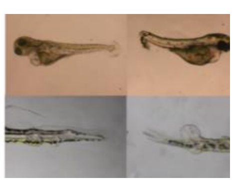
Mortality vs. AuNP Exposures

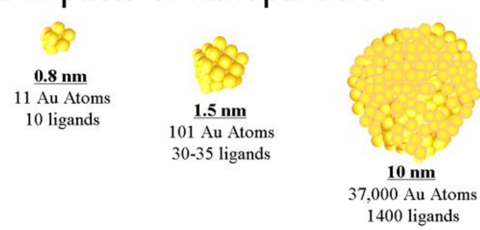


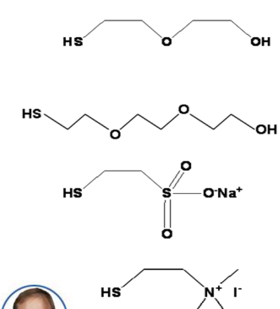
ACS Nano **2011,** *5*, 4688

31

Example: Design principles from a systematic study of biological impacts of nanoparticles







malformations	malformations	NA
toxic	toxic	

ACS Nano **2011**, 4688-97

32

Progress toward design of safer nanoparticles

Design of safer nanomaterials (P4,P12) →

- Avoid incorporation of toxic elements (Cd^{2+}, Ag^{+}, Zn^{2+})
- Analogies to materials with similar attributes (CNM vs. PAHs and soot)
- Use SARs to design effective, safer materials that possess desired physical properties

Current understanding: Toxicity is dictated by the overall dimensions and surface coating

Three classes of exceptions so far:

- Leachable toxic ions
- Catalytic surfaces if the surface isn't completely coated
- Material that doesn't remain soluble/dispersed

Chem. Rev. **2007**, *107,* 2228
ACS Nano **2008**, *2*, 395

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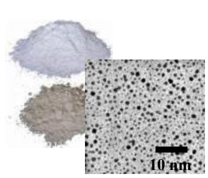
What about products (e.g. textiles) that contain nanomaterials?



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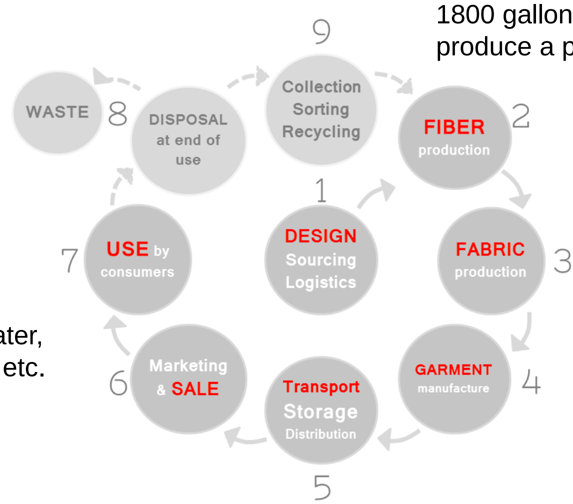
Life cycle impacts of the textile industry

8000 chemicals used
1800 gallons of water to produce a pair of jeans



Laundry:
Energy, water, detergent, etc.

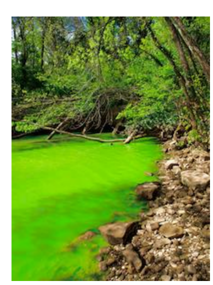
35

Potential benefit: Reducing impacts in the use phase (laundry)

Water use: Nearly a trillion gallons (1.5 million Olympic-sized swimming pools) used in US annually, about 25% of household use

CO_2 emissions (mostly drying): 179 million metric tons/year (~25% of the CO_2 emitted by passenger vehicles in the US)

Detergents:
Lifecycle impacts


Eutrophication

https://center.sustainability.duke.edu/resources/green-facts-consumers/heating-water-really-biggest-laundry-impact (accessed July 2015).

36

Consumer need: Eliminate/control/prevent persistent odor

Polyester is the dominant fabric: 60% of textiles

Persistent odor commonly develops in polyester garments.
- Bacteria thrive on, and in, the synthetic fibers.
- Synthetics absorb fatty acids (from sweat) that are food for bacteria
- Bacteria become trapped in fibers – not washed out

What are the consequences of persistent odor?
- Undesirable for consumers
- Drives many consumer behaviors
  - More washing
  - More (harsh) detergent use
  - Dispose of garment

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Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

If nanotechnology could reduce odor build up in clothing, and reduce the need for laundering, in which phases of the lifecycle would impacts be reduced? (multiple correct answers possible)

- Manufacturing
- Transportation
- Use
- Disposal
- Reuse/recycle

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What about the use of nanosilver as an anti-odor fabric coating?

- **Silver has been used as for centuries:** dishware, cutlery, jewelry, coins and medical applications
- If nanoAg prevents persistent odor and extends garment life, **impacts can be reduced** throughout the lifecycle

- Can nanoAg products be developed to **enhance performance and minimize impact**?
- If so, is there a **net environmental benefit** across the lifecycle of using nanoAg compared to traditional approaches?

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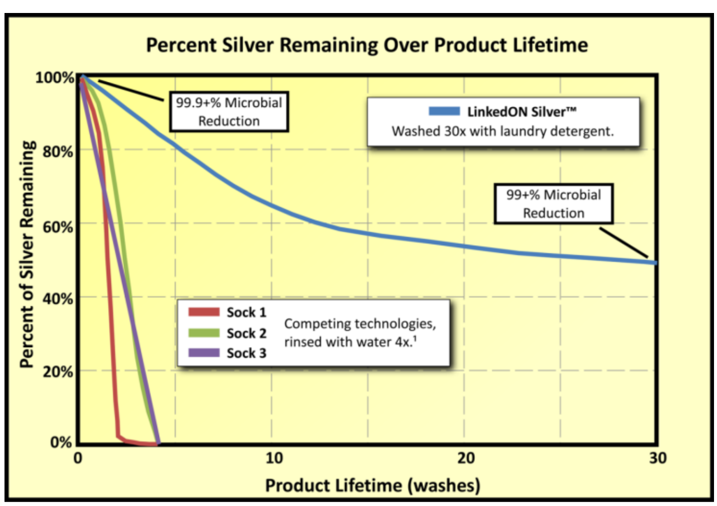
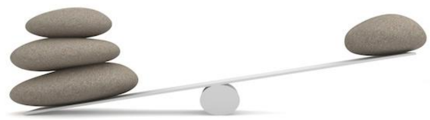
Silver was lost rapidly from early nanosilver products



Environ. Sci. Technol., ***2008, 42, 4133*** and data from Dune Sciences

40

Benefits, impacts and net environmental benefit



LC impacts of textiles and nanoAg vs. functional performance

$$\text{Impact-benefit ratio} = \frac{\text{Life cycle impacts}}{\text{Functional performance benefits}}$$

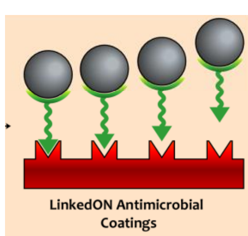
L.M. Gilbertson, et al. *Chem. Soc. Rev.* **2015**, *44*, 5758-5777.

Measure and compare benefits as well as impacts
Need to understand the chemistry of these products

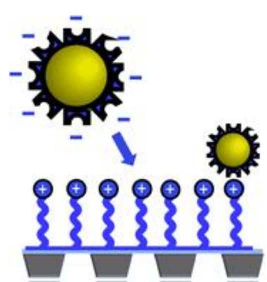
41

Better linking reduces impacts and improves functional performance

Treated fabrics kill more than 99% of bacteria after more than 50 launderings



Less silver used (20 ppm) and much less is released



What happens to silver during use?

DUNE SCIENCES

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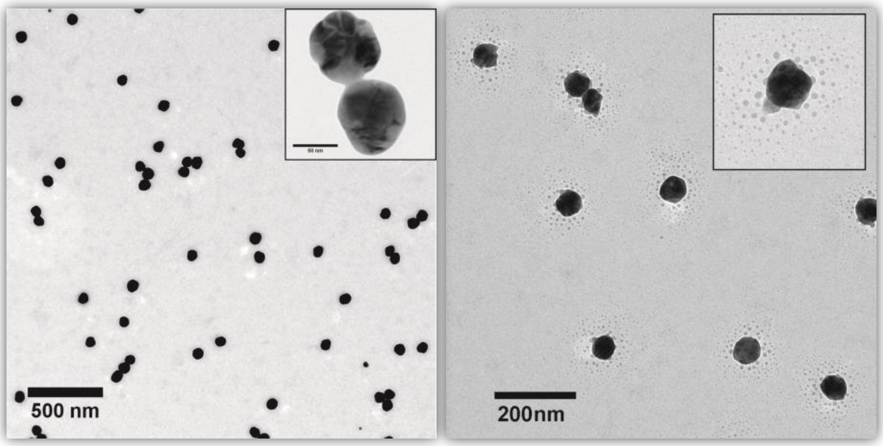
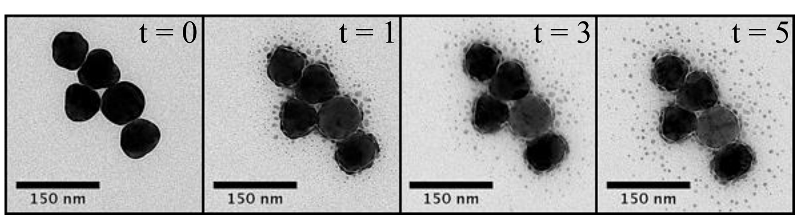
A surprise – Ag NPs transform tethered to the grid under ambient lab conditions

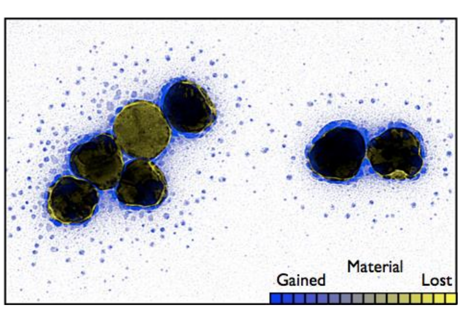


Glover, R.D.; Miller, J.M.; Hutchison, J.E. *ACS Nano*, **2011**, *5*, 8950

43

Direct observation of nanoparticle transformations at 100% RH over five weeks





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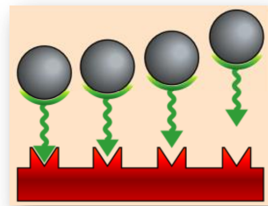
Lessons for design from nanoSilver studies

The different forms of silver (ions, nanoparticles and bulk metal) interconvert

Initial form of silver in the product may not dictate potential hazards



Design of next generation product:

- Attach silver so that it is not released from the product
- Incorporate silver at the **lowest** possible loading to attain performance – nanoparticles are well suited for this
- Analyze benefits and compare to alternatives

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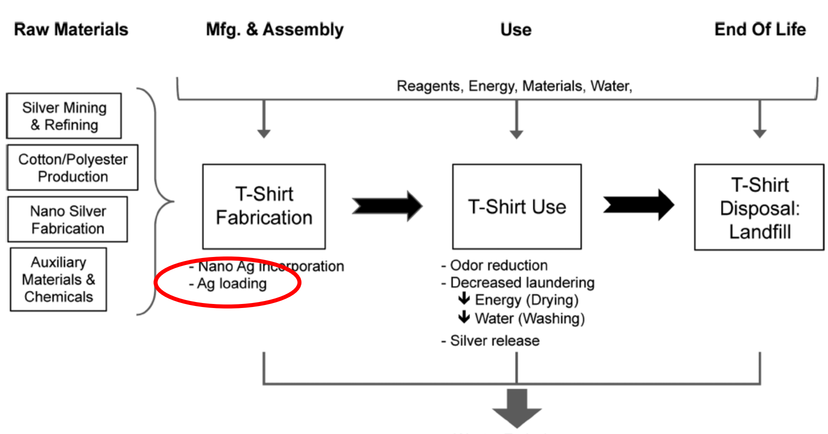
Lifecycle thinking - use the minimum effective amount of silver to maximize the net environmental benefit



"Life Cycle Payback Estimates of Nanosilver Enabled Textiles under Different Silver Loading, Release, and Laundering Scenarios Informed by Literature Review," A. L. Hicks et al. *Environ. Sci. Technol.* **2015**, 7529–7542.

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Lifecycle thinking - use the minimum effective amount of silver to maximize the net environmental benefit

"…suggests that shifts in consumer laundering behavior, including replacement of RE with HE appliances and line drying or reduced laundering as a function of the nanoenabled properties of the textile, ***has the potential to significantly reduce laundering impacts, and subsequently GHGs***. While the median concentration of silver (**10,800 µg silver/g textile**) was used for these impact assessments, there is potential for the impacts to shift as technology improves (e.g., attachment method, functional efficacy)."

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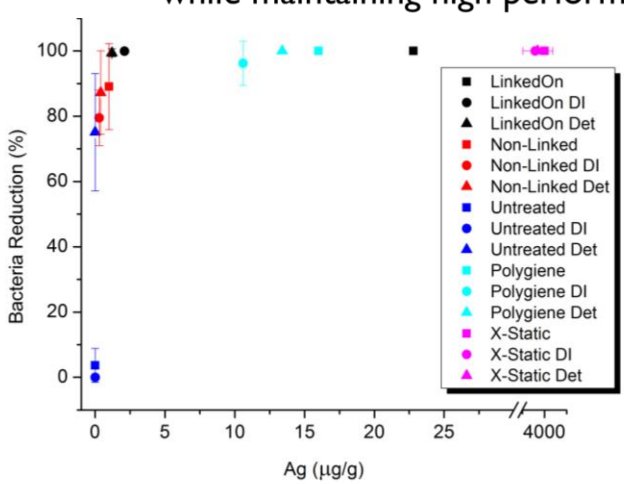
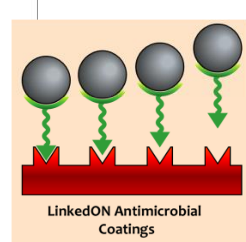
Lower Ag loadings decrease impacts while maintaining high performance





"Potential Environmental Impacts and Antimicrobial Efficacy of Silver- and Nanosilver-Containing Textiles," Reed, R.B et al., *Environ. Sci. Technol.*, **2016**, *50*, 4018–4026.

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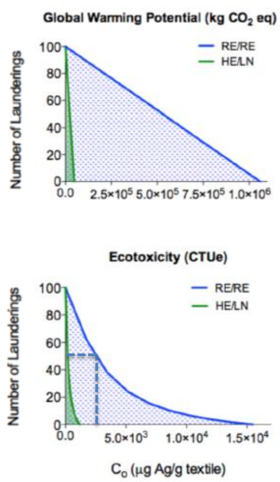
Determining the environmental payback – net benefit



Comparing nanoAg to conventional t-shirts

- Lifespan of conventional t-shirt assumed to be 100 washes
- Graphs show number of launderings of nanoAg t-shirt to still gain an environmental benefit

Example

- For ecotoxicity, at 2500 ppm, would have to wash < 50 times to accrue a net benefit
- At 20 ppm, the shirts are nearly equal. If consumers wash 50% less, impacts are cut nearly in half

Environ. Sci. Technol. **2015**, 7529–7542.

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Product developed to eliminate and prevent odor buildup in active wear

Product development was catalyzed by feedback from studies that assessed benefits and impacts and identified hotspots for innovation

Keys to success:

- Seek chemical understanding to guide design for performance
- Use lifecycle thinking to identify ways to reduce impacts
- Enhance performance
- Reduce impact
- Compare to conventional alternatives

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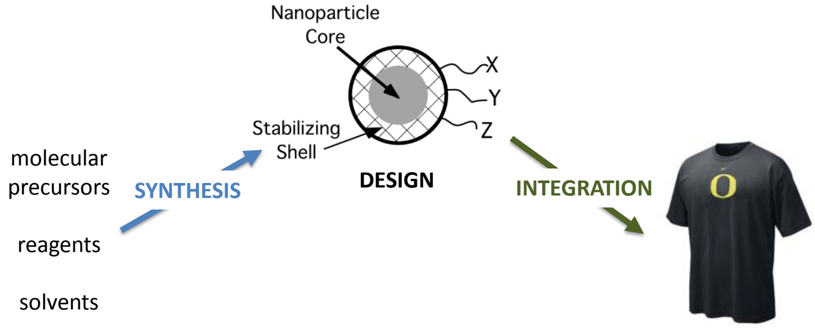
Summary



- Green chemistry improves performance and lowers impact
- Molecular-level understanding is essential to successful design
- Life cycle thinking is a powerful approach to identify avenues for product development
- It is important to consider performance as well as impacts, so that we do not sacrifice needed performance

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Reviews and Perspectives

Hutchison, J.E. "The road to sustainable nanotechnology: Challenges, progress and opportunities," *ACS Sustain. Chem. Eng.* **2016**, 4, 5907–5914.

Gilbertson, L. M. et al. "Designing Nanomaterials to Maximize Performance and Minimize Undesirable Implications Guided by the Principles of Green Chemistry," *Chem. Soc. Rev.* **2015**, 44, 5758-5777.

Hutchison, J. E. "Greener Nanoscience: A Proactive Approach to Advancing Applications and Reducing Implications of Nanotechnology," *ACSNano* **2008,** *2*, 395-402.

Dahl, J. et al. "Toward Greener Nanosynthesis," *Chem. Rev.* **2007**, *107*, 2228-2269.

McKenzie, L. C.; Hutchison, J. E. "Green Nanoscience," *Chimica Oggi (Chemistry Today)* **2004**, *22*, 30-33. September 2004.

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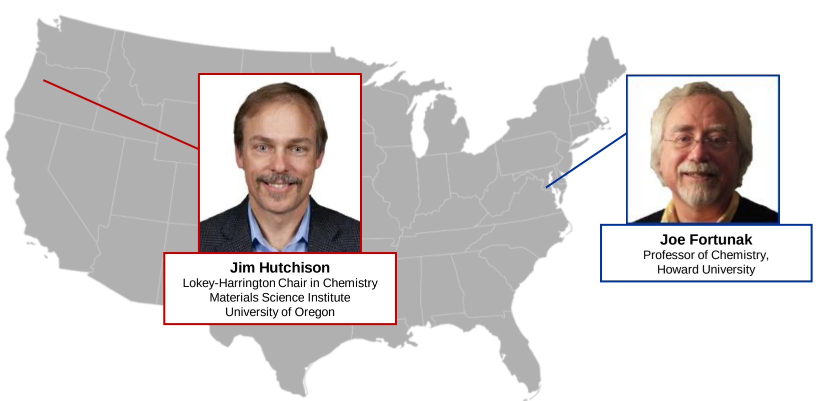

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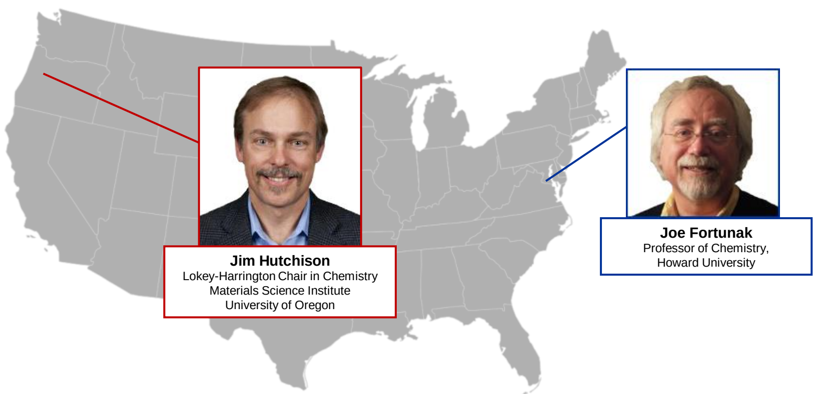

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